

Table 1 Selected X-ray Crystallographic Data

Cocrystal	1	2	3
Empirical formula	C ₁₂₉ H ₂₀₀ N ₄ O _{37.50}	C ₆₅ H ₁₀₂ N ₂ O ₂₀	C ₄₉ H ₆₄ N ₁ O _{27.55}
M _r	2406.93	1231.49	1107.81
Space group	P-1	P21/c	C2/c
a/Å	12.137(5)	18.022(4)	29.602(8)
b/Å	16.978(7)	16.787(3)	15.909(4)
c/Å	31.818(13)	22.439(5)	25.288(7)
α/°	92.2253(6)	90	90
β/°	90.065(6)	104.818(2)	97.868(4)
γ/°	93.959(6)	90	90
V/Å ³	6536(5)	6563(2)	11769(6)
T/K	173(2)	173(2)	100(2)
λ/Å	0.71073	0.71073	0.7749
d _c /g cm ⁻³	1.223	1.246	1.250
Z	2	4	8
GOF	1.054	1.032	1.408
R ₁ [I > 2σ(I)] ^a	0.0914	0.0524	0.1178
wR ₂ (all data) ^b	0.2927	0.1619	0.3655

^a R₁ = Σ||F_o - |F_c|| / Σ |F_o|. ^b wR₂ = [Σ w(F_o² - F_c²)² / Σ w(F_o²)²]^{1/2}.